

Quantum annealing with Jarzynski equality

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We show a practical application of the Jarzynski equality in quantum computation. Its implementation may open a way to solve combinatorial optimization problems, minimization of a real single-valued function, cost function, with many arguments. We consider to incorporate the Jarzynski equality into quantum annealing, which is one of the generic algorithms to solve the combinatorial optimization problem. The ordinary quantum annealing suffers from non-adiabatic transitions whose rate is characterized by the minimum energy gap Δ of the quantum system under consideration. The quantum sweep speed is therefore restricted to be extremely slow for the achievement to obtain a solution without relevant errors. However, in our strategy shown in the present study, we find that such a difficulty would not matter.

Quantum computer is believed to be able to solve intractable problems on classical computer by use of superposition, tunneling effect and entanglement attributed to quantum nature. This fascinating device is attracted to researchers and studied from both aspects of the fundamental interests of quantum nature and its application. The intractable problems we wish to solve are often closely related to efficiency for cost and time in industry and distribution systems to gain convenience in our daily life. The efforts in both of the theoretical and experimental approaches have culminated to realize quantum computer, which can mitigate the difficulties to solve such hard problems. Hundreds of hard problems are found in optimization problem, which is a kind of the problems to minimize or maximize a real single-valued function of multivariables called the cost function. The cases in which variables take discrete values are known as combinatorial optimization, whose well-known instances are satisfiability problems, exact cover, maximum cut, Hamilton graph, and traveling salesman problem [1, 2]. Most of the interesting optimization problems belong to the hard class in which the best known algorithms cost exponentially long time as a function of the system size (the number of degrees of freedom representing the cost function). Therefore one desires quantum computation, which enables us to solve such hard optimization problems by an algorithm employing quantum nature. One of the generic algorithms proposed as part of such efforts is quantum annealing (QA) [3–5]. In QA, we introduce artificial degrees of freedom of quantum nature, noncommutative operators, which induce quantum fluctuations to drive the system as

$$H(t) = f(t)H_0 + \{1 - f(t)\}H_1, \quad (1)$$

where H_0 is the classical Hamiltonian consisting of diagonal elements, which express the cost function. Here $f(t)$ is assumed to be a monotonically increasing function satisfying $f(0) = 0$ and $f(\tau) = 1$. The quantum annealing starts from a single pure state, the ground state of H_1 , which is chosen to be trivially given as

$|\Psi(0)\rangle = \sum_{\{\sigma\}} |\sigma\rangle / \sqrt{N}$, where N characterizes the system size of the optimization problem. The adiabatic theorem guarantees that we can reach a nontrivial ground state of H_0 after quantum dynamics with sufficiently slow speed as $1/\tau_c \sim \Delta_{\min}^2$, where τ means the annealing time, and Δ is the energy gap of the instantaneous quantum system as in Eq. (1) [5, 6]. However QA does not work well in a reasonable time, since we require extremely slow control, for the cases in which the quantum system as in Eq. (1) has a minimum energy gap vanishing as $\Delta_{\min} \sim \exp(-\alpha N)$ for increasing the system size N [7, 8]. The quantum annealing is a very generic technique but has such a bottleneck.

To overcome the above difficulty, we bring another theoretical piece from non-equilibrium statistical physics, the Jarzynski equality (JE), in the present study [9, 10]. The Jarzynski equality is written by an well-known expression as,

$$\langle e^{-\beta W} \rangle = \frac{Z_\tau(\beta)}{Z_0(\beta)}, \quad (2)$$

where the angular brackets denote the average over all realizations in a predetermined process starting from an initial equilibrium state and W is the work done during the process. The partition functions for the initial and final Hamiltonians are written as $Z_0(\beta)$ and $Z_\tau(\beta)$ with inverse temperature β , respectively. We here recall the formulation of JE for classical systems on a heat bath [10]. Let us consider a thermal nonequilibrium process in a finite-time schedule $0 \leq t \leq \tau$. Thermal fluctuations can be simulated by the master equation. We employ discrete time expressions and write $t_{k+1} - t_k = \delta t$, $t_0 = 0$ and $t_n = \tau$. The probability that the system is in a state σ_k at time t_k is denoted as $P(\sigma_k; t_k)$. The transition probability per unit time δt is defined as $M(\sigma_{k+1}|\sigma_k; t_k)$. In the original formulation of JE, the work is defined as the energy difference merely attributed to the change of the Hamiltonian, but we can construct JE also in the case of changing the inverse temperature by defining the work as $-\beta W(\sigma_k; t_k) = -(\beta(t_{k+1}) - \beta(t_k))E(\sigma_k)$, where $E(\sigma)$

is the value of the cost function (classical Hamiltonian H_0) for the specific state σ . The left-hand side of JE can be expressed as

$$\langle e^{-\beta W} \rangle = \sum_{\{\sigma_k\}} \prod_{k=0}^{n-1} \left\{ e^{-\beta W(\sigma_{k+1}; t_k)} e^{\delta t M(\sigma_{k+1} | \sigma_k; t_k)} \right\} \times \tilde{P}(\sigma_0; t_0), \quad (3)$$

where $\tilde{P}(\sigma_0; t_0)$ denotes the initial equilibrium distribution. The initial condition is set to the equilibrium distribution. If the transition term $\exp(\delta t M(\sigma_{k+1} | \sigma_k; t_k))$ is removed in Eq. (3), JE is trivially satisfied because the summation of $-\beta W(\sigma_{k+1}; t_k)$ over k yields $-(\beta(t_n) - \beta(t_0))E(\sigma_0)$. A non-trivial aspect of JE is in the insertion of the transition term, which does not alter the conclusion. From Eq. (3), it is straightforward to prove JE. This is the case for classical systems on a heat bath, not for quantum systems. One may think the above classical equality is not available for the application to QA. Nevertheless we can apply the classical JE to QA by aid of the classical-quantum mapping [11].

The classical-quantum mapping leads us to a special quantum system, in which the (instantaneous) equilibrium state of the above stochastic dynamics can be expressed as a ground state. A general form of such a special quantum Hamiltonian is

$$H_q(\sigma' | \sigma; t) = \delta_{\sigma', \sigma} - e^{\beta(t) H_0(\sigma')/2} M(\sigma' | \sigma; t) e^{-\beta(t) H_0(\sigma)/2}. \quad (4)$$

This Hamiltonian has the ground state as $|\Psi_{\text{eq}}(t)\rangle = \sum_{\sigma} e^{-\frac{\beta(t)}{2} H_0(\sigma)} |\sigma\rangle / \sqrt{Z(t)}$. It is clear that the quantum expectation value of a physical quantity $A(\sigma)$ by $|\Psi_{\text{eq}}(t)\rangle$ is equal to the thermal expectation value for the same quantity. The ground state energy is 0, which can be explicitly shown by the detailed-balance condition. On the other hand, the excited states have positive-definite eigenvalues, which can be confirmed by the Perron-Frobenius theorem.

In the above special quantum system, we can treat a quasi-equilibrium stochastic process as an adiabatic quantum-mechanical dynamics in QA. Let us consider QA for the above special quantum system by setting the parameter corresponding to the temperature $T \rightarrow \infty$ ($\beta \rightarrow 0$). This condition gives the trivial ground state with uniform linear combination, similarly to the ordinary QA. If we tune $T \rightarrow 0$ very slowly, one can obtain the ground state for H_q , which expresses the very low-temperature equilibrium state for H_0 , the cost function of the optimization problem that we wish solve. Notice that we use a single quantum state during the above procedure, not an ensemble assumed in the ordinary formulation in JE.

Let us construct a protocol with the same spirit as JE by using the special quantum system. Initially we prepare the trivial ground state with the uniform linear combination as in the ordinary QA. From the point

of view of the classical-quantum mapping, this initial state expresses the high-temperature equilibrium state $|\Psi_{\text{eq}}(t_0)\rangle \propto e^{-\beta(t_0) H_0(\sigma)/2} |\sigma\rangle$ with $\beta(t_0) \ll 1$. We introduce the exponentiated work operator $W(\sigma_k; t_k) = \exp(-(\beta(t_{k+1}) - \beta(t_k)) H_0(\sigma_k)/2)$. It looks like a non-unitary operator, but we can construct this operation by considering an extended quantum system as discussed later. If we apply $W(\sigma_k; t_k)$ to the quantum wave function $|\Psi_{\text{eq}}(t_k)\rangle$, the state is changed into a state corresponding to the equilibrium distribution with the inverse temperature $\beta(t_{k+1})$. When the time-evolution operator $U(\sigma' | \sigma; t_{k+1}) = \exp(-i \delta t H_q(\sigma' | \sigma; t_{k+1})/\hbar)$ is applied, this state does not change, since it is the ground state of $H_q(\sigma' | \sigma; t_{k+1})$. The obtained state after the repetition of the above procedure is

$$|\Psi(t_n)\rangle \propto \prod_{k=0}^{n-1} \{ W(\sigma_{k+1}; t_k) U_{k+1}(\sigma_{k+1} | \sigma_k; t_k) \} |\Psi_{\text{eq}}(t_0)\rangle. \quad (5)$$

This is essentially of the same form as Eq. (3). Instead of the exponentiated matrix of $\delta t M(\sigma_{k+1} | \sigma_k; t_k)$, we use the time-evolution operator $U(\sigma_{k+1} | \sigma_k; t_k)$ here. After the system reaches the state $|\Psi(t_n)\rangle$, we measure the obtained state by the projection onto a specified state σ' . The probability is then given by $|\langle \sigma' | \Psi(t_n) \rangle|^2$, which means that the ground state we wish to find is obtained with the probability proportional to $\exp(-\beta(t_n) H_0)$, since $|\Psi(t_n)\rangle \propto |\Psi_{\text{eq}}(t_n)\rangle$. If we carry out the above procedure up to $\beta(t_n) \gg 1$, we can efficiently obtain the ground state of H_0 . This is called the quantum Jarzynski annealing (QJA) in the present paper.

It may seem to be unnecessary to apply the time-evolution operator $U(\sigma_{k+1} | \sigma_k; t_k)$, which expresses the change between states by quantum fluctuations, at the middle step between the operations of the exponentiated work operators $W(\sigma_{k+1}; t_k)$. The time-evolution operator does not mean an artificial control but describes the change by quantum nature during quantum computation. Let us remember the nontrivial point of JE. Even if we allow transitions between the exponentiated work, JE holds as in Eq. (3).

We emphasize the following three points. First, the scheme of QJA does not rely on the quantum adiabatic control. The computational time does not depend on the energy gap. Therefore QJA does not suffer from the energy-gap closure differently from the ordinary QA. It is thus important to estimate the required computational cost from the number of the unitary gates for the implementation of QJA as will be discussed below. Second, from a point of JE, the result is independent of the schedule to tune the parameter, τ , in the above manipulations. Third, we do not need the repetition of the pre-determined process to deal with all fluctuations in the nonequilibrium-process average as in the ordinary JE, since the classical ensemble is mapped to the

quantum wave function. We operate the above procedure to a single quantum system in principal. Notice that, since we need a kind of practical techniques to realize QJA, several-time repetitions of experiments should be demanded since the result by quantum measurement should be probabilistic. However we should emphasize that this point is not related with the theoretical property of JE attributed to rare events, necessity of all the realizations during the nonequilibrium process, but it comes from quantum nature.

According to the property of JE, we can expect that QJA finds the ground state following the Gibbs-Boltzmann factor independently of annealing schedules. In contrast, without the multiplication of the exponentiated work, slow quantum control is necessary to efficiently find the ground state according to the ordinary QA. Let us take a simple instance to search the minimum from a one-dimensional random potential, which is formulated as the Hamiltonian $H_0 = -\sum_{i=1}^N V_i |i\rangle\langle i|$. Here V_i denotes the potential energy at site i and chosen randomly. By the linear schedule for tuning the parameter β from 0 to 100, we apply QA without exponentiated work operations and QJA to the above system. Figure 1 shows the comparison between the probability for finding the ground state with $N = 50$ sites by QA and QJA with different schedules $\tau = 1, 10$ and 100. The plots for QJA (upper curves) are fixed along the reference curves (dashed curves) representing the instantaneous Gibbs-Boltzmann factor. In other words, QJA does not depend on τ , which characterizes the schedule of quantum computation. In contrast, QA (lower curves) needs sufficiently slow decrease of quantum fluctuations to efficiently find the ground state.

To perform QJA, we need to implement the exponentiated work operation $W(\sigma_k; t_k) = \exp(-(\beta(t_{k+1}) - \beta(t_k))H_0(\sigma_k)/2)$, which looks like a non-unitary operator. To implement this operation, we consider a quantum state with an ancilla qubit (another two-level quantum system) as $|\Psi, \phi_1\rangle = |\Psi\rangle \otimes |\phi_1\rangle$, where ϕ_1 is assumed to take 0 and 1 [12]. Initially we set $|\Psi, \phi_1 = 0\rangle$, which is called the computational state below. It is convenient to assume the case that $H_0(\sigma) > 0$ for any states. Let us define the following “unitary” operator for the enlarged quantum system as

$$\begin{aligned} W_{\text{unit.}} &= \sum_{\sigma} |\sigma\rangle\langle\sigma| \otimes \begin{pmatrix} \sqrt{y(\sigma)} & \sqrt{1-y(\sigma)} \\ -\sqrt{1-y(\sigma)} & \sqrt{y(\sigma)} \end{pmatrix} \\ &\equiv I_{\sigma} \otimes Y_1, \end{aligned} \quad (6)$$

where $y(\sigma) = \exp(-\delta\beta H_0(\sigma))$. We can obtain the weighted quantum system by applying this operator to the computational state as $\sqrt{y(\sigma)}|\Psi, \phi_1 = 0\rangle$. In that sense, we can regard $W_{\text{unit.}}$ as the exponentiated work operation $W(\sigma_k; t_k)$ for the quantum state $|\Psi, \phi_1 = 0\rangle$ as above shown for the case in which we increase β monotonically. We can explicitly evaluate each probability am-

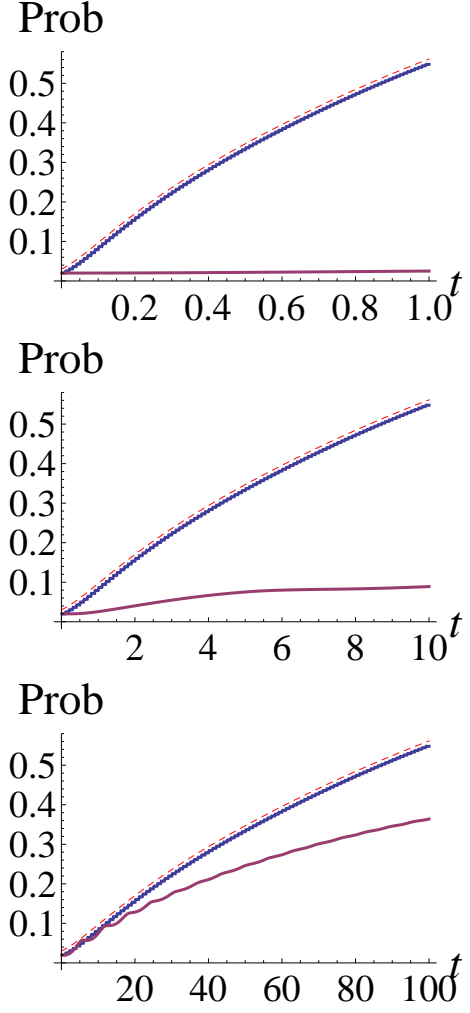


FIG. 1: (color online) Quantum Jarzynski annealing and quantum annealing for the one-dimensional random-potential problem. The probabilities for obtaining the ground state by both of the methods are plotted for $\tau = 1, 10$, and 100 from top to bottom. The dashed curves denote the instantaneous Gibbs-Boltzmann factor for reference. The upper solid curves (blue curves) representing the results by QJA are fixed to these reference curves, while the lower ones (red ones) express the time-dependent results by the ordinary QA.

plitude of $W_{\text{unit.}}|\Psi, \phi_1 = 0\rangle$ as

$$\langle\Psi, 0|W_{\text{unit.}}|\Psi, 0\rangle = \sqrt{y(\sigma)} \quad (7)$$

$$\langle\Psi, 1|W_{\text{unit.}}|\Psi, 0\rangle = \sqrt{1-y(\sigma)} \quad (8)$$

When we consider measurements of the quantum state, $\sqrt{1-y(\sigma)}|\Psi, \phi_1 = 1\rangle$ is regarded as an undesired error state in our computation. We have to bound the error probability $p_{\text{error}} = 1 - y(\sigma)$. To decrease the error probability and to avoid negative numbers in the square root, we here demand $p_{\text{error}} \sim \delta\beta \max_{\sigma} H(\sigma) \ll 1$.

In QJA, to gain the relevant weight for the ground state of H_0 , we have to increase a parameter correspond-

ing to the inverse temperature up to $\beta(t_n)\epsilon \sim 1$, where ϵ is the minimum energy gap of the “classical” Hamiltonian H_0 (usually given by the energy unit). Therefore the step of QJA, which corresponds to the step number of the work operation $W_{\text{unit.}}$, is necessary up to $n \equiv \beta(t_n)/\delta\beta \sim 1/\epsilon\delta\beta$. As a result, the computational time (the step number of the exponentiated work operation) should become longer as $n \sim 1/\epsilon\delta\beta = \max_{\sigma} H_0(\sigma)/\epsilon p_{\text{error}}$ to make the error probability p_{error} lower in our strategy. However the computational time for QJA does not depend on the detailed structure of the cost function.

Since $\delta\beta$ is bound, we have to prepare an enlarged quantum state with n ancilla qubits as $|\Psi, \phi_1, \dots, \phi_n\rangle$ to obtain the quantum state with the relevant weight after n -step exponentiated work operation as detailed below. The computational state of QJA in this case is $|\Psi, 0, \dots, 0\rangle$. The other states as $|\Psi, 1, 0, \dots, 0\rangle$, $|\Psi, 0, 1, \dots, 0\rangle$, etc. such that several ancilla qubits are flipped as $\phi_i = 1$ are regarded as the error states similarly to the above simple case. To gain the weight up to $\exp(-\beta(t_n)H_0)$, we consider the n -step exponentiated work operations as $I_{\sigma} \otimes Y_1 \otimes I_2 \otimes \dots \otimes I_n$, $I_{\sigma} \otimes I_1 \otimes Y_2 \otimes I_3 \otimes \dots \otimes I_n$, \dots and $I_{\sigma} \otimes I_1 \otimes \dots \otimes I_{n-1} \otimes Y_n$, where I_j denotes the identity matrix. We then obtain the desired state $|\Psi, 0, 0, \dots, 0\rangle$ after measurements with the weight as $\exp(-\beta(t_n)H_0) = (1 - p_{\text{error}})^n$. The weights for the other states, the error states, are given as $p_{\text{error}}(1 - p_{\text{error}})^{n-1}$ for $|\Psi, 1, 0, \dots, 0\rangle$ and $p_{\text{error}}^2(1 - p_{\text{error}})^{n-2}$ for $|\Psi, 1, 1, 0, \dots, 0\rangle$ and so on. Therefore we can obtain the desired state by repetition of the experiments when we consider the realistic implementation of QJA in quantum computation. The demanded number of the repetition of the same experiments is evaluated as $1/(1 - p_{\text{error}})^n \sim 1 + \max_{\sigma} H_0(\sigma)/\epsilon$, which does not depend on the choice of p_{error} .

We here summarize the results of the above estimations. We tune the value of $p_{\text{error}} \ll 1$ (for instance, $p_{\text{error}} = 0.01$) in order to efficiently yield the desired quantum state as $\exp(-\beta(t_n)H_0)|\Psi, 0, \dots, 0\rangle$. Simultaneously the computational time for QJA is determined as $n \sim \max_{\sigma} H_0(\sigma)/\epsilon p_{\text{error}}$ (in the case $p_{\text{error}} = 0.01$, $n \sim 100 \max_{\sigma} H_0(\sigma)/\epsilon$). Also the number of the repetition of the same experiments can be estimated as $\sim 1 + \max_{\sigma} H_0(\sigma)/\epsilon$. Even if the maximum value of the cost function becomes larger by increase of the system size as $\max_{\sigma} H(\sigma)/\epsilon = N^r$ where r is an arbitrary positive value, both of the computational time and the number of the ancilla qubits do not diverge exponentially, since $n \sim N^r/p_{\text{error}}$. The repetition of the experiments can also be reduced to a moderate value as $\sim 1 + N^r$.

We consider an application of JE to quantum computation as QA to solve the optimization problems by using the classical-quantum mapping. The classical-quantum mapping enables us to imitate pseudo-thermal processes

in quantum computation. As we expected, this protocol keeps the quantum system to express the equilibrium state for the instantaneous inverse temperature. To decrease some errors occurring after the exponentiated work operation and measurements, we can not increase rapidly the inverse temperature to obtain the ground state and we need additional qubits. Nevertheless the cost for the realization of QJA in quantum computation does not diverge exponentially, which is the essentially different point from the ordinary QA and other quantum algorithms. The key point of QJA is that we need another resource like a “memory” in quantum computation instead of cut “time”. Fortunately, the amount of necessary memory (ancilla qubits) as well as the computational time for implementation of QJA does not diverge exponentially by the increase of the system size N . Thus the results by QJA shown here imply that we may overcome the difficulties in hard optimization problems and solve them in a reasonable time. The present results are preliminary but we should clarify the efficiency for several interesting hard problems we wish to solve in the future study [13]. We hope that QJA becomes one of the basic algorithms using the quantum nature.

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